

INTRODUCTION

We are particularly interested in the doping and substitution effects of boron on adamantane with a view to tuning the absorption range to give potential application in optoelectronics and photocatalysis. We used time-dependent density-functional theory (TDDFT) to examine these effects. Optical and electronic properties have been calculated for a range of substituted systems. For one, the HOMO-LUMO energy gap was found to be lowered while the absorption spectrum has shifted to within the red region of the visible spectrum. This poster will outline our work to date and make suggestions for synthetic investigation

COMPUTATIONAL METHODS

Five set of adamantane species; ADM, ADM 1HB, ADM 2HB, ADM 2B-1H, ADM 2B-2H and ADM 2B were design by doping and substitution at different carbon positions as shown in figure 1. Different computational methods including HF, MP2 and the hybrid dispersion-corrected DFT functional M06-2X were used to compute the optimized structure and frequencies using different basis sets such as 6-31G*, 6-311G* and aug-cc-pVTZ. The electronics and optical properties were computed at same level of theory using TD-DFT. All the computational calculation were performed using Gaussian 16 computation software package.

RESULTS

Optimized Geometries at M062X/631G*

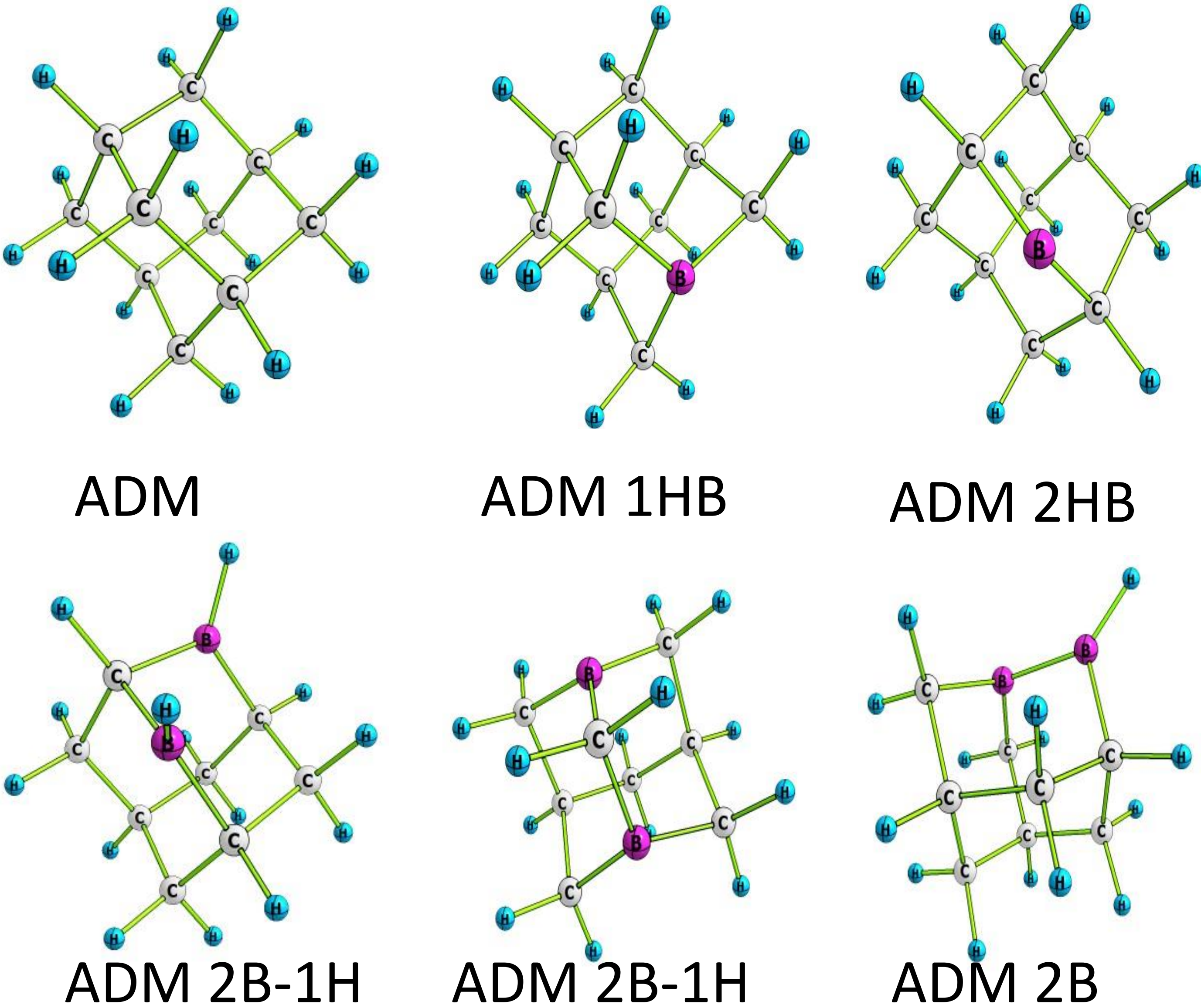
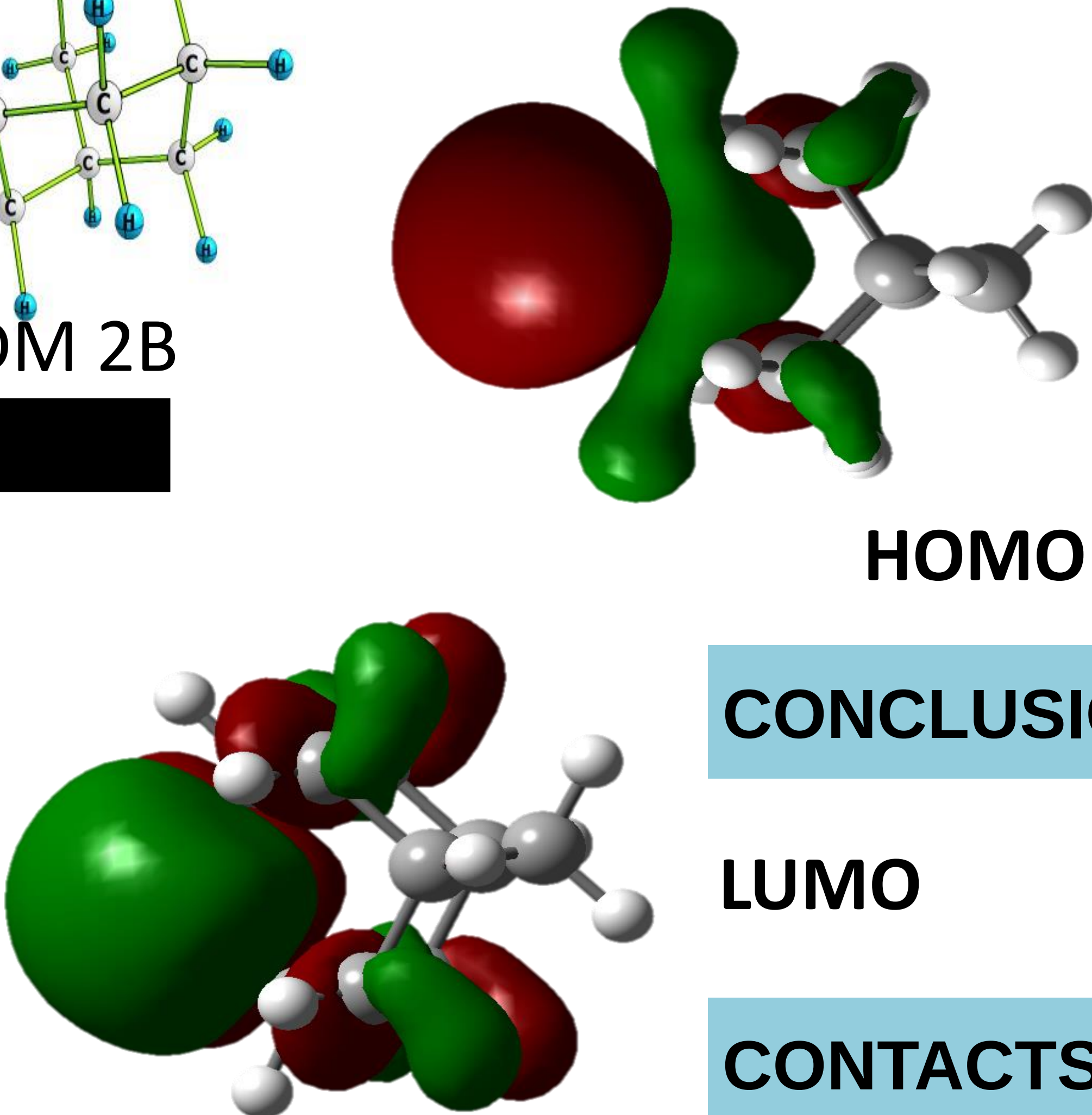


Figure 1: Optimized geomitries

Selected parameters of the optimized molecules at M062X/631G* level of theory

Species	C-H	C-C	C-B	C-C-H	C-C-C	C-B-C	H-C-B	H-C-C-H	C-C-C-B	H-C-C-B	H-C-B-C
ADM	1.09801	1.53719	0	109.961	109.748	0	0	58.916	0	0	0
ADM 1HB	1.09695	1.53906	1.56969	109.202	109.466	31.765	115.52	59.35	119.412	180	172.626
ADM 2HB	1.09551	1.5364	1.55953	110.383	109.932	32.46	115.288	60.56	128.228	64.835	180
ADM 2B-1H	1.0928	1.53434	1.57771	108.965	110.451	32.803	113.448	56.987	129.177	63.154	175.449
ADM 2B-2H	1.09285	1.54143	1.57458	108.426	110.148	32.182	115.408	58.468	126.079	178.8.03	173.199
ADM 2B	1.0953	1.53853	1.58033	108.733	111.274	32.593	112.812	55.764	124.299	179.716	173.608

HOMO-LUMO Diagram of ADM-2HB



CONCLUSION

LUMO

CONTACTS

Optical Properties computed using TD-DFT @B3LYP/6-311G

Specie	Wavelength (nm)	Absorbance	Energy (eV)
ADM	165.17	0.0046	7.5062
ADM 1HB	221.76	0.0031	5.5908
ADM 2HB	642.03	0.0018	1.9311
ADM 2B-1H	288.57	0.0045	4.3965
ADM 2B-2H	268.45	0.004	4.6285
ADM 2B	293.72	0.0059	4.2211

The results revealed the doping effects of bron on adamantane by tuning its characteristic into semiconductor. ADM-2H in particular has shifted its molecular spectrum into the visible region confirming its eligibility in photocatalysis and elcetronics applications.

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